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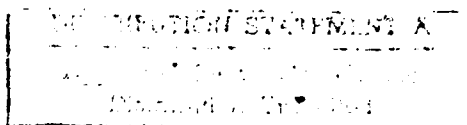
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**On the Computation of Impasse Points of
Quasilinear Differential Algebraic Equations¹**

BY

PATRICK J. RABIER AND WERNER C. RHEINBOLDT²



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1. Introduction.

Many applications in science and engineering involve mixed systems of differential and algebraic equations (DAE's). For some examples see, for instance, the monograph [BCP89]. It is hardly surprising that such systems share many properties with ordinary differential equations (ODE's). In fact, recent existence theories ([Rh91], [RR91a], [RR91b]) have shown that, in general, a DAE can be reduced locally to an (explicit) ODE on some submanifold of the space of unknown variables.

However, despite the strong analogy between DAE's and ODE's, important differences exist. For instance, from the fact that DAE's are reducible to ODE's only on some submanifold of the solution space it follows that solutions of a DAE can pass only through points on such a submanifold; that is, its initial values must satisfy certain compatibility conditions. Beyond this, solutions of DAE's may exhibit features that solutions of explicit ODE's cannot possess. For instance, the simple problem

$$x_1^2 + x_2 = 0, \quad \dot{x}_2 = 1, \quad x(0) = (1, -1)$$

has the unique solution $x(t) = ((1-t)^{1/2}, t-1)$ which cannot be continued beyond $t = 1$ despite the fact that $x(1) = (0, 0)$ and $\lim_{t \rightarrow 1^-} x(t) = x(1)$ exist. This situation would be impossible for solutions of explicit ODE's.

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In the electrical engineering literature such type of points have been called impasse points (see e.g. [C69] or [CD89] where also other references are given). Although they have no analog in connection with explicit ODE's they are closely related to the "singular points" of implicit ODE's. In [Ra89] the most often encountered type of such singularities for implicit ODE's was analyzed, called there standard singular points. In a recent paper [RR92a] it was shown that the geometric reduction theory for DAE's presented in [RR91b] allows for a generalization of the results in [Ra89] to so-called standard impasse points of quasilinear DAE's.

The aim of this article will be to show that the theory of [RR92] leads naturally to the development of a computational procedure for the explicit computation of standard impasse points of quasilinear DAE's. For this we outline, in Sections 2 and 3, briefly and without proof, some of the relevant results for singular ODE's and DAE's from the cited earlier papers. Then Section 4 presents the details of the computational algorithm and finally in Section 5 we give some numerical examples which show the effectivity of the process.

2. Singular Points of ODE's.

Definition 2.1. Consider a quasilinear problem

$$(2.1) \quad B(y)\dot{y} = H(y), \quad y(0) = y_0$$

where $B : \mathcal{D} \rightarrow \mathcal{L}(\mathbb{R}^n)$ and $H : \mathcal{D} \rightarrow \mathbb{R}^n$ are C^1 on some open set $\mathcal{D} \subset \mathbb{R}^n$. A point $y \in \mathcal{D}$ is a regular point of (2.1) if $\text{rank } B(y) = n$ and a singular point if $\text{rank } B(y) < n$ but y is a limit point of regular points of (2.1).

Clearly, for a regular point $y_0 \in \mathcal{D}$ the initial value problem (2.1) has a unique solution in a neighborhood of y_0 . But already simple examples show that the behavior of the solutions of (2.1) in a neighborhood of a singular point y_0 may vary strongly with the type of singularity encountered there. A partial classification of singularities which will be sufficient for our purposes is given next:

Definition 2.2. (i) A singular point $y \in \mathcal{D}$ of the ODE in (2.1) r -singular if

$$(2.2) \quad \dim \ker B(y) = r.$$

(ii) A 1-singular point is called basic if

$$(2.3) \quad H(y) \notin \text{rge } B(y).$$

(iii) A basic 1-singular point is a standard singular point if

$$(2.4) \quad DB(y)(u, u) \notin \text{rge } B(y), \quad \forall u \in \ker B(y) \setminus \{0\}.$$

We summarize here briefly the theory developed in [Ra89] for the case of standard singular points (see also [RR92]). With a standard singular point y_0 as starting point the initial value problem (2.1) cannot have a C^1 solution $y : J \rightarrow \mathcal{D}$ on an open interval J containing the origin. In fact, this would require that $B(y_0)\dot{y}(0) = H(y_0)$ which contradicts (2.3). Thus at a standard singular point we may expect at best “one-sided” solutions in the following sense:

Definition 2.3. With a standard singular point $y_0 \in \mathcal{D}$ as starting point a solution of the initial value problem (2.1) is any continuous function $y : J \rightarrow \mathcal{D}$ defined on an interval $J = [0, T)$ or $J = (-T, 0]$ for some $T > 0$ which is of class C^1 on $J^0 = J \setminus \{0\}$ and satisfies $y(0) = y_0$ and $B(y(t))\dot{y}(t) = H(y(t))$ for $t \in J^0$.

With

$$(2.5) \quad \alpha(y)(u, v) = (v^T H(y)) (v^T DB(y)(u, u))$$

the two conditions (2.3) and (2.4) for a standard singular point y are equivalent to

$$(2.6) \quad \alpha(y)(u, v) \neq 0, \quad \forall u \in \ker B(y) \setminus \{0\}, \quad v \in \ker B(y)^T \setminus \{0\}.$$

Since (2.5) is a continuous, quadratic form in u and in v its value must be either positive or negative for all pairs of nonzero vectors $u \in \ker B(y)$, $v \in \ker B(y)^T$ if only this holds for one such pair of vectors.

The principal existence result for solutions near standard singular points can now be phrased as follows (see [Ra89, Theorem 5.1]) :

Theorem 2.1. *Let $y_0 \in \mathcal{D}$ be a standard singular point of the ODE in (2.1). Then the initial value problem (2.1) has exactly two solutions which are both defined on $J = [0, T)$ or on $J = (-T, 0]$ for some $T > 0$ depending upon $\alpha(y_0)(u, v) > 0$ or $\alpha(y_0)(u, v) < 0$, respectively, for some pair of nonzero vectors $(u, v) \in \ker B(y) \times \ker B(y)^T$. Moreover, $\|\dot{y}(t)\|$ tends to infinity as $t \in J \setminus \{0\}$ tends to zero.*

Theorem 2.1 implies that a solution of (2.1) starting at some regular point can reach a standard singular point y_0 at some later time only if the form (2.5) is negative at y^0 . Standard singular points y_0 with positive $\alpha(y_0)$ obviously can never be reached in increasing time. Thus, in view of the theorem, the following notation is appropriate:

Definition 2.4. *A standard singular point y_0 of (2.1) is accessible or inaccessible if $\alpha(y_0)(u, v) < 0$ or $\alpha(y_0)(u, v) > 0$, respectively, for some pair of nonzero vectors $(u, v) \in \ker B(y) \times \ker B(y)^T$.*

The theorem asserts that accessible standard singular points are reached in finite time by trajectories emanating elsewhere in \mathcal{D} . Since these trajectories cannot be continuously extended beyond these points, they represent “catastrophes” for the solutions of (2.1) and standard ODE-solvers fail near such points. It can also be shown (loc. cit.) that no small perturbation of the initial condition (and/or of B or H) can affect the eventual encounter of such points.

Standard singular points are analogous to limit points of parametrized nonlinear equations

$$F(z, \lambda) = 0.$$

Suppose, indeed, that $F : \mathcal{D} \rightarrow \mathbb{R}^n$ is of class C^1 on some open set $\mathcal{D} \subset \mathbb{R}^n \times \mathbb{R}^1$ and that $z : J \rightarrow \mathbb{R}^n$ is a C^1 mapping on an open interval J such that $(z(\lambda), \lambda) \in \mathcal{D}$ and

$F(z(\lambda), \lambda) = 0$ for $\lambda \in J$. Then

$$(2.7) \quad \begin{pmatrix} D_z F(z(\lambda), \lambda) & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} z'(\lambda) \\ \lambda' \end{pmatrix} + \begin{pmatrix} D_\lambda F(z(\lambda), \lambda) \\ 1 \end{pmatrix} = 0,$$

where primes indicate differentiation with respect to λ , and hence (2.7) is an ODE of the quasi-linear form (2.1). The singular points of (2.7) are exactly those $(z, \lambda) \in \mathcal{D}$ for which $\text{rank } D_z F(z, \lambda) < n$; that is, which are foldpoints of F with respect to λ (see e.g. [Rh86]). The simplest foldpoints are the limit points for which $\dim \ker D_z F(z, \lambda) = 1$ and $D_\lambda F(z, \lambda) \notin \text{rge } D_z F(z, \lambda)$. Obviously, these two properties correspond to the conditions (2.2) and (2.3) and it is readily checked that (2.4) holds exactly for the simple limit points of F (with respect to λ), (see e.g. [Rh86]).

Foldpoints of a parametrized nonlinear system are typically computed by solving a suitably augmented form of the system. It is natural to consider the same approach for the computation of singular points of ODE's.

Let $y = y(t)$ be a C^1 -solution of (2.1) and suppose that a C^1 function $\tau : \mathbb{R}^1 \rightarrow \mathbb{R}^1$ with strictly positive derivative is used to define a transformation $t = \tau(s)$ of the independent variable t . Then $\eta(s) = y(\tau(s))$ satisfies

$$B(\eta) \frac{d\eta}{ds} = \frac{d\tau}{ds} H(\eta).$$

By Theorem 2.1 the derivative dy/dt becomes infinite when the solution approaches a standard singular point y^* . This suggests that τ should be chosen such that $d\tau/ds$ tends to zero as we approach y^* but $d\eta/ds$ remains bounded. For instance, we may wish to specify τ implicitly by using a normalization $c^T(d\eta/ds) = 1$ with a suitable vector $c \in \mathbb{R}^n$.

This normalization may be obtained by means of an augmented system of the form

$$(2.8) \quad \begin{pmatrix} B(y) & -H(y) \\ c^T & 0 \end{pmatrix} \begin{pmatrix} v(y) \\ \gamma(y) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

where $c \in \mathbb{R}^n$ is chosen such that at a point $\tilde{y} \in \mathcal{D}$ under consideration the matrix of (2.8) is nonsingular. Certainly, such an augmentation can be found if and only if \tilde{y} is either a regular point of (2.1) or a basic 1-singular point.

Hence the matrix of (2.8) remains nonsingular for all y in some open neighborhood $\mathcal{U} \subset \mathcal{D}$ of \tilde{y} whence for fixed $y \in \mathcal{U}$ the solution $(v(y), \gamma(y)) \in \mathbb{R}^{n+1}$ of (2.8) is unique. Obviously we have $v(y) \neq 0$ for all $y \in \mathcal{U}$ and $\gamma(y) \neq 0$ for all regular points $y \in \mathcal{U}$ of (2.1). Moreover, because of (2.3) we see that $\gamma(y^*) = 0$ at any basic 1-singular point $y^* \in \mathcal{U}$.

For any regular point $y_0 \in \mathcal{U}$ the initial value problem (2.1) has a unique, local C^1 -solution $y : [0, T) \rightarrow \mathcal{U}$ for some $T > 0$. Suppose that $\gamma(y_0) > 0$. Then $\gamma(y(t)) > 0$ for $0 \leq t < T$ and the initial value problem

$$(2.9) \quad \frac{dt}{ds} = \gamma(y(t)), \quad s \in [0, T), \quad t(0) = 0,$$

has a unique, monotonically increasing solution $\tau : [0, \sigma) \rightarrow \mathbb{R}^1$ with $0 < \sigma < T$. Hence, as desired, τ defines a transformation of the independent variable t of (2.1). As before, we set

$$(2.10) \quad \eta(s) = y(\tau(s)), \quad s \in [0, \sigma), \quad \eta(0) = y_0.$$

Together with (2.9) the chain rule provides that

$$(2.11) \quad \frac{d\eta}{ds}(s) = \gamma(\eta(s)) \frac{dy}{dt}(\tau(s)), \quad s \in [0, \sigma)$$

whence by (2.1) and (2.8) it follows that

$$B(y(t)) \left[\gamma(y(t)) \frac{dy}{dt}(t) - v(y(t)) \right] = 0, \quad 0 \leq t < T;$$

and therefore, by (2.10) and (2.11), that

$$(2.12) \quad \frac{d\eta}{ds}(s) = v(\eta(s)), \quad \eta(0) = y_0, \quad s \in [0, \sigma).$$

Proposition 2.1. Suppose that the solution $y = y(t)$ of (2.1) tends to some standard singular point $y^* \in \mathcal{U}$ and hence has been extended to a maximal interval $[0, T^*)$ such that $\lim_{t \rightarrow T^*} y(t) = y^*$. (Necessarily, y^* is a basic 1-singular point since the matrix of the augmentation (2.8) is invertible at y^* by hypothesis). Then (i) there exists $\sigma^* < \infty$ such that the solution $t = \tau(s)$ of (2.9) is defined for $s \in [0, \sigma^*)$ and that $\lim_{s \rightarrow \sigma^*} \tau(s) = T^*$. (ii) The solution of (2.12) is defined and of class C^1 on $[0, \sigma^* + \epsilon)$ for some $\epsilon > 0$. (iii) If, in addition y^* is a standard singular point, then $\gamma(\eta(s))$ changes sign as s crosses σ^* .

Proof: Let J denote the set of all $\bar{\sigma}$ such that there exists a C^1 -solution of (2.9) for $s \in [0, \bar{\sigma})$ satisfying $0 \leq \tau(s) < T^*$ on that interval. Clearly, J is not empty and hence $\sigma^* = \sup\{\bar{\sigma} : \bar{\sigma} \in J\}$ is well defined. Thus there exists a C^1 -solution of (2.9) for $s \in [0, \sigma^*)$ satisfying $0 \leq \tau(s) < T^*$ on this interval. In order to show that $\lim_{s \rightarrow \sigma^*} \tau(s) = T^*$ note that τ remains monotonically increasing on $[0, \sigma^*)$ and hence that $\lim_{s \rightarrow \sigma^*} \tau(s) = \tau^* \leq T^*$ exists. Suppose that $\tau^* < T^*$. Then, by the continuity of γ , the compactness of $y([0, \tau^*])$, and the fact that $\gamma(y(t)) > 0$ for $t \in [0, T^*)$, it follows that there exists a positive constant γ_0 for which $\gamma(y(t)) \geq \gamma_0$ in $[0, T^*)$. This implies that $\sigma^* < \infty$, for otherwise $\tau(s) \geq \gamma_0 s$ for $s \in [0, \infty)$ and hence $\lim_{s \rightarrow \infty} \tau(s) = \infty$ in contradiction with $0 \leq \tau(s) \leq \tau^* < \infty$ for $s \in [0, \sigma^*) = [0, \infty)$. But now, by setting $\tau(\sigma^*) = \tau^*$, we can define a continuous extension of τ to some interval $[0, \sigma^* + \epsilon]$ with sufficiently small $\epsilon > 0$ such that $0 \leq \tau(s) < T^*$. Thus, assuming $\tau^* < T^*$ we obtain a contradiction with the maximality of σ^* . This shows that $\tau^* = T^*$.

The above arguments show only that $\sigma^* \leq \infty$, but we can show that $\sigma^* < \infty$. In fact, assume, to the contrary, that $\sigma^* = \infty$ so that η is defined in $[0, \infty)$. Since by construction $c^T v(\eta(s)) \equiv 1$ it follows from (2.12) that $c^T(d\eta/ds)(s) \equiv 1$ whence $c^T \eta(s) = c^T y_0 + s$. This implies that $\lim_{s \rightarrow \infty} c^T \eta(s) = \infty$ and hence also that $\lim_{s \rightarrow \infty} \|\eta(s)\| = \infty$. But then we arrive at a contradiction since $\|\eta(s)\| = \|y(\tau(s))\|$ and $\|y(t)\|$ is bounded on the compact interval $[0, T^*]$. This proves (i).

It follows from (i) that (2.12) has a unique solution η for $s \in [0, \sigma^*)$ and $\eta(\sigma^*) = y^*$ defines a continuous extension of η . Therefore, the solution of (2.12) can be extended to a larger interval $[0, \sigma^* + \epsilon)$ with some $\epsilon > 0$ as claimed in (ii).

As noted earlier, we have $\gamma(\eta(s)) > 0$ for $0 \leq s < \sigma^*$ and $\gamma(\eta(\sigma^*)) = \gamma(y^*) = 0$. Thus σ^* is the first zero of $\gamma(\eta(s))$ in $[0, \sigma^* + \epsilon)$. If now y^* is a standard singular point, $\gamma(\eta(s))$ must change sign as s crosses σ^* . For this note that by differentiation of

$$B(\eta(s))v(\eta(s)) = \gamma(\eta(s))H(\eta(s)), \quad s \in [0, \sigma^*],$$

together with $\gamma(y^*) = 0$ we obtain for all $h \in \mathbb{R}^n$ that

$$DB(y^*)(h, v(y^*)) + B(y^*)Dv(y^*)h = (D\gamma(y^*)h)H(y^*).$$

For $h = v(y^*) \neq 0$ and any nonzero vector $w \in \ker B(y^*)^T$ it follows from (2.5) and (2.6) that

$$D\gamma(y^*)v(y^*) = \frac{w^T DB(y^*)(v(y^*), v(y^*))}{w^T H(y^*)} = \frac{\alpha(y^*)(v(y^*), w)}{(w^T H(y^*))^2} \neq 0.$$

Since $d(\gamma \circ \eta)/ds(\sigma^*) = D\gamma(y^*)v(y^*)$, this proves that indeed $(\gamma \circ \eta)(s)$ must change sign as s crosses σ^* . \square

Altogether, therefore, by solving (2.12) and monitoring the first sign change of $\gamma(\eta(s))$ we can calculate σ^* and hence $y^* = \eta(\sigma^*)$. The value of T^* is then given by

$$(2.13) \quad T^* = \int_0^{\sigma^*} \gamma(\eta(s))ds,$$

which follows directly from (2.9) and $\lim_{s \rightarrow \sigma^*} \eta(s) = T^*$.

The augmentation procedure described here is designed to work in the neighborhood of a standard singular point. But in practice, also higher order singularities $y^* \in \mathcal{D}$ are encountered where the matrix of the simple augmented system (2.8) becomes singular. In order to avoid difficulties near such points, we may work with an overdetermined augmented system of the form

$$(2.14) \quad \begin{pmatrix} B(y) & -H(y) & E \\ C^T & 0 & 0 \end{pmatrix} \begin{pmatrix} V(y) \\ w(y)^T \\ Z(y)^T \end{pmatrix} = \begin{pmatrix} 0_{n \times q} \\ I_q \end{pmatrix}.$$

Here, for given q , $1 < q \leq n$, the matrices E and C have dimension $n \times (q - 1)$ and $n \times q$, respectively, and, correspondingly, in the solution, $V(y)$, $w(y)$, and $Z(y)$ are blocks of size $n \times q$, $q \times 1$, and $q \times (q - 1)$, respectively. As before, the matrices E and C are chosen such that at some “current” point $y_c \in \mathcal{D}$ the matrix of (2.14) is nonsingular and hence remains nonsingular for all y in some open neighborhood $\mathcal{U}_c \subset \mathcal{D}$ of y_c . Thus, for each $y \in \mathcal{U}_c$ the solution of (2.14) is unique. Clearly, for sufficiently large q this can be accomplished irrespective of $\dim \ker B(y_c)$ and even in the case when $H(y_c) \in \text{rge } B(y_c)$; (except when $H(y_c) = 0$; but see Remark 2.1 further below).

We summarize some basic properties of the augmentation (2.14):

Proposition 2.2. *For given $q > 1$ and $y \in \mathcal{U}_c$ the solution of (2.14) satisfies*

$$(2.15) \quad \dim \ker B(y) = \dim \ker (w(y), Z(y)),$$

and $\text{rank } Z(y) = q - 1$ implies that $\text{rank } (B(y), -H(y)) = n$. The converse holds if $H(y) \notin \text{rge } B(y)$ (and hence y is a basic 1-singular point).

Proof: Generally, for $y \in \mathcal{U}_c$ we have

$$(2.16) \quad B(y)V(y) = (H(y), -E)(w(y), Z(y))^T,$$

as well as $\text{rank } V(y) = q$ (since $C^T V(y) = I_q$) and $\text{rank } (H(y), -E) = q$ (since the matrix of (2.14) is invertible) which together imply the first assertion. Indeed, since both $V(y)$ and $(H(y), -E)$ are $n \times q$, $q \leq n$, and have maximum rank q , we infer from (2.16) that

$$\dim \ker B(y)V(y) = \dim \ker (w(y), Z(y))^T = \dim \ker (w(y), Z(y))$$

(recall that $(w(y), Z(y))$ is $q \times q$). Moreover, using again the fact that $\ker V(y) = \{0\}$, we see that

$$(2.17) \quad \dim \ker B(y)V(y) \leq \dim \ker B(y).$$

Thus, to complete the proof of (2.15), it suffices to show that the converse inequality of (2.17) holds. This follows at once if we can show that $\ker B(y) \subset \text{rge } V(y)$. For this let $u \in \ker B(y)$, so that

$$(2.18) \quad \begin{pmatrix} B(y) & -H(y) & E \\ C^T & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ 0_{1 \times 1} \\ 0_{(q-1) \times 1} \end{pmatrix} = \begin{pmatrix} 0_{n \times 1} \\ C^T u \end{pmatrix}.$$

On the other hand, $C^T V(y) = I_q$ implies that $C^T V(y) C^T u = C^T u$ and hence, by (2.16), that

$$(2.19) \quad \begin{pmatrix} B(y) & -H(y) & E \\ C^T & 0 & 0 \end{pmatrix} \begin{pmatrix} V(y) C^T u \\ w(y)^T C^T u \\ Z(y)^T C^T u \end{pmatrix} = \begin{pmatrix} 0_{n \times 1} \\ C^T u \end{pmatrix}.$$

But the systems (2.18) and (2.19) have the same right hand side, and hence, because the matrix is invertible, the solutions are identical whence, in particular, $u = V(y) C^T u$ and therefore $u \in \text{rge } V(y)$.

If $\text{rank } Z(y) = q - 1$ then $\text{rge } EZ^T = \text{rge } E$. Therefore, $\text{rge } E \subset \text{rge } (B(y), -H(y))$ and hence $\text{rge } (B(y), -H(y), E) = \text{rge } (B(y), -H(y))$ which for $\text{rank } (B(y), -H(y)) < n$ contradicts the nonsingularity of the matrix of (2.14).

To prove that, conversely, $\text{rank } (B(y), -H(y)) = n$ and $H(y) \notin \text{rge } B(y)$ imply $\text{rank } Z(y) = q - 1$ suppose that $H(y) \notin \text{rge } B(y)$ and $\text{rank } Z(y) \leq q - 2$, so that $\dim \ker Z(y)^T \geq 2$. Let u_α , $\alpha = 1, 2$ be two linearly independent vectors in $\ker Z(y)^T$. By (2.16) we have

$$B(y)V(y)u_\alpha = (w(y)^T u_\alpha)H(y), \quad \alpha = 1, 2$$

and hence $w(y)^T u_\alpha = 0$, $\alpha = 1, 2$, since $H(y) \notin \text{rge } B(y)$. Thus $u_\alpha \in \ker (w(y), Z(y))^T$, $\alpha = 1, 2$. By (2.15) the linear independence of the two vectors implies that $\dim \ker B(y) \geq 2$, which in turn implies that $\text{rank } (B(y), -H(y)) < n$. \square

For $y \in \mathcal{U}_c$ and any nonzero vector $a(y) \in \ker Z(y)^T$ we have

$$(2.20a) \quad B(y)v(y) = \gamma(y)H(y), \quad c(y)^T v(y) = a(y)^T a(y),$$

$$(2.20b) \quad v(y) = V(y)a(y), \quad c(y) = Ca(y), \quad \gamma(y) = w(y)^T a(y).$$

This has the general form of (2.8), and as before, $\gamma(y) = 0$ implies that $B(y)$ is singular. But, the converse is not necessarily true. Moreover, the vector $a(y)$ must depend smoothly on y . This is easily guaranteed as long as $\text{rank } Z(y) = q - 1$ but is not generally feasible unless we drop the assumption that $a(y) \neq 0$. Let $Z^i(y)$ denote the $(q - 1) \times (q - 1)$ submatrix obtained from $Z(y)$ by deleting the i -th column. Then the vector

$$(2.21) \quad a(y) = (a_1(y), \dots, a_q(y))^T, \quad a_i(y) = (-1)^i \det Z^i(y), \quad i = 1, \dots, q,$$

obviously depends smoothly on y and satisfies $Z(y)^T a(y) = 0$, (see e.g. [S73], Appendix II). Moreover, we have $a(y) \neq 0$ exactly if $\text{rank } Z(y) = q - 1$.

For this choice of $a(y)$ the following result holds:

Proposition 2.3. *For $y \in \mathcal{U}_c$ and with the vectors (2.21) consider the relations (2.20). Then $\gamma(y) = 0$ exactly if $B(y)$ is singular.*

Proof: If $\gamma(y) = 0$ then either $\text{rank } Z(y) < q - 1$ in which case, by (2.15), $B(y)$ is singular, or $\text{rank } Z(y) = q - 1$ whence $a(y) \neq 0$ and thus also $v(y) \neq 0$ which together with $B(y)v(y) = 0$ implies again that $B(y)$ is singular. Conversely, suppose that $B(y)$ is singular. In the case $\text{rank } Z(y) = q - 1$, we have again $v(y) \neq 0$ and Proposition 2.2 ensures that $H(y) \notin \text{rge } B(y)$. Thus the first equation (2.20a) leads to a contradiction unless $\gamma(y) = 0$. On the other hand for $\text{rank } Z(y) < q - 1$ we necessarily have $\gamma(y) = 0$ because $a(y) = 0$ in that case. \square

By Proposition 2.2 we see that when $B(y)$ is singular and $H(y) \in \text{rge } B(y)$ then necessarily $\text{rank } Z(y) < q - 1$. Such points are evidently not standard impasse points, and hence constitute “higher” singularities. Our choice (2.21) of $a(y)$ evidently transforms these points into equilibrium points of the dynamic system (2.12) with v as in (2.20b).

Computationally the simplest case arises with $q = 2$ where (2.14) has the form

$$(2.22) \quad \begin{pmatrix} B(y) & -H(y) & e \\ c_1^T & 0 & 0 \\ c_2^T & 0 & 0 \end{pmatrix} \begin{pmatrix} v_1(y) & v_2(y) \\ w_1(y) & w_2(y) \\ z_1(y) & z_2(y) \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Hence, the vector (2.21) becomes here $a(y) = (-z_2(y), z_1(y))$ and we obtain

$$(2.23) \quad \begin{aligned} v(y) &= z_2(y)v_1(y) - z_1(y)v_2(y), \\ \gamma(y) &= z_2(y)w_1(y) - z_1(y)w_2(y), \\ c(y) &= z_2(y)c_1(y) - z_1(y)c_2(y). \end{aligned}$$

Proposition 2.3 implies that $\gamma(y)$ does not vanish on a trajectory terminating at a singular point $y^* \in \mathcal{U}_c$. Obviously (2.22) has the same general form as the simple augmentation (2.8) and the computational procedure is the same as before, namely, we form and solve the explicit equation (2.12). The only difference is that the normalization condition now involves the nonconstant vector $c(y)$ while in (2.8) this vector was constant.

The constancy of c was used to prove that for a basic 1-singular point there exists $\sigma^* < \infty$ such that the solution $t = \tau(s)$ of (2.9) is defined for $[0, \sigma^*)$ and that $\lim_{s \rightarrow \sigma^*} \tau(s) = T^*$. The result is easily extended to the case when c depends on y . For this note that the proof of the existence of $\sigma^* \leq \infty$ carries over verbatim and is irrespective of the singularity encountered at y^* ; all that is needed is that the matrix (2.22) be invertible at y^* . Now if y^* is a basic 1-singular point and $\sigma^* = \infty$ we conclude from $c(\eta(s))^T v(\eta(s)) = \|a(y)\|_2^2$ that $c(y^*)^T v(\eta(s)) \geq \epsilon > 0$ for all s close to σ^* . Indeed, $\text{rank } Z(y^*) = q - 1$ by Proposition 2.2 and hence $a(y^*) \neq 0$. In other words, for sufficiently large s it follows that $c(y^*)^T (d\eta/ds)(s) \geq \epsilon$ and therefore that $c(y^*)^T \eta(s) \geq \epsilon(s - s_0) + c(y^*)^T \eta(s_0)$ for $s \geq s_0$ and s_0 large enough. As before, this contradicts the boundedness of $\|\eta(s)\|$ for $s \geq 0$.

If y^* is a standard singular point, then $\gamma(\eta(s))$ changes sign as s crosses σ^* . Obviously, if y^* is not a basic 1-singular point then we can no longer ascertain that $\sigma^* < \infty$.

Remark 2.1 The matrix of any augmentation (2.14) and, in particular, that of (2.8) or (2.22), will be singular at any point $y \in \mathcal{U}_c$ where $H(y) = 0$; that is, at any stationary (equilibrium) point of the autonomous ODE (2.1). This reflects the fact that any regular stationary point can be reached only in infinite time and hence our scale-transformation must become indetermined along such trajectories. Clearly, the natural resolution of this difficulty is to make the system (2.1) *non-autonomous* by adding the equation $\dot{t} = 1$.

3. Singular Points of DAE's.

In this section we turn to differential-algebraic systems of the following form:

Definition 3.1. *The equation*

$$(3.1) \quad A(x)\dot{x} = G(x),$$

with C^2 mappings $A : \mathcal{D} \rightarrow \mathcal{L}(\mathbb{R}^n)$ and $G : \mathcal{D} \rightarrow \mathbb{R}^n$ on some open set $\mathcal{D} \subset \mathbb{R}^n$ is a quasilinear DAE on \mathcal{D} if

$$(3.2) \quad G(x) \in \text{rge } A(x), x \in \mathcal{D} \implies \text{rank } A(x) = r$$

and if the mapping

$$(3.3) \quad (x, p) \in \mathcal{D} \times \mathbb{R}^n \longmapsto A(x)p - G(x) \in \mathbb{R}^n,$$

is a submersion.

The submersion property of (3.3) requires that for every $(x, p) \in \mathcal{D} \times \mathbb{R}^n$ the mapping

$$(3.4) \quad (h, k) \in \mathbb{R}^n \times \mathbb{R}^n \longmapsto (DA(x)h)p + A(x)k - DG(x)h \in \mathbb{R}^n,$$

is onto (see e.g. [AMR88]). As a consequence the set

$$(3.5) \quad M = \{(x, p) \in \mathcal{D} \times \mathbb{R}^n : A(x)p - G(x) = 0\}$$

is a closed n -dimensional C^2 -submanifold of $\mathcal{D} \times \mathbb{R}^n$.

In [RR91b] a geometric procedure was developed for reducing an implicit DAE $F(x, \dot{x}) = 0$ to a system of ODE's on a manifold locally near a point $(x^0, p^0) \in F^{-1}(0)$. A simplified version of this reduction process for quasilinear DAE's (3.1) is given in [RR92]. In that case the reduction is local only in the first variable due to the linearity of the equation in \dot{x} . We summarize briefly this process for (3.1).

Set

$$(3.6) \quad W = \{x \in \mathcal{D} : G(x) \in \text{rge } A(x)\},$$

so that $(x, p) \in M$ if and only if $x \in W$ and hence $W = \pi(M)$ where $\pi : \mathcal{D} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ is the projection onto the first factor. Under the conditions of Definition 3.1 it can be shown (see [RR92], Proposition 3.1) that W is an r -dimensional C^2 -submanifold of \mathcal{D} and that W is closed in \mathcal{D} if the set $\{x \in \mathcal{D} : \text{rank } A(x) = r\}$ is closed in \mathcal{D} .

For any C^1 -solution $x : J \rightarrow \mathcal{D}$ of (3.1) on an open interval $J \subset \mathbb{R}^1$ we must have $x(t) \in W$ for $t \in J$ and thus $(x(t), \dot{x}(t)) \in TW$ for all $t \in J$ where we view here the tangent bundle TW as a subset of $T\mathbb{R}^n = \mathbb{R}^n \times \mathbb{R}^n$. Hence $(x(t), \dot{x}(t)) \in M$ implies that $(x(t), \dot{x}(t)) \in TW \cap M$ for all $t \in J$. The desired reduction of (3.1) now requires a (local) characterization of $TW \cap M$.

For this let $x^0 \in W$. Then there exist open subsets $\mathcal{U} \subset W$ and $\mathcal{V} \subset \mathbb{R}^r$ and a C^2 -map $\varphi : \mathcal{V} \rightarrow \mathbb{R}^n$ which is a diffeomorphism of \mathcal{V} onto \mathcal{U} . In other words, φ^{-1} is a chart of W at x^0 .

Evidently, \mathcal{U} and \mathcal{V} may be chosen small enough such that there is a linear subspace $Z^0 \subset \mathbb{R}^n$ which complements $\text{rge } A(\varphi(y))$ for all $y \in \mathcal{V}$. Let P^0 be the projection of \mathbb{R}^n onto $\text{rge } A(x^0)$ along Z^0 and L^0 any linear isomorphism from $\text{rge } A(x^0)$ onto \mathbb{R}^r . Then $L^0 \circ P^0$ is a linear isomorphism of $\text{rge } A(\varphi(y))$ onto \mathbb{R}^r for all $y \in \mathcal{V}$ and it follows that

$$\{(x, p) \in TW \cap M, x \in \mathcal{U}\} \Leftrightarrow \begin{cases} x = \varphi(y), p = D\varphi(y)q, \\ B(y)q - H(y) = 0, \end{cases}$$

where we have set

$$(3.7) \quad B(y) = L^0 P^0 A(\varphi(y)) D\varphi(y), \quad H(y) = L^0 P^0 G(\varphi(y)).$$

Evidently, the operators B and H map into $\mathcal{L}(\mathbb{R}^r)$ and \mathbb{R}^r , respectively, and are of class C^1 .

If the interval of definition $J \subset \mathbb{R}^1$ of the solution is restricted to ensure that $x(J) \subset \mathcal{U}$ and therefore that $(x(t), \dot{x}(t)) \in TW \cap M$ and $x(t) \in \mathcal{U}$ for all $t \in J$, then the C^1 function

$$(3.8) \quad y : J \rightarrow V, \quad y(t) = \varphi^{-1} \circ x(t),$$

is a C^1 -solution of the equation

$$(3.9) \quad B(y)\dot{y} = H(y),$$

called the reduction of (3.1) near x^0 . Conversely, for any C^1 -solution $y : J \rightarrow \mathcal{V}$ of (3.9) the function $x(t) = \varphi \circ y(t)$ is a C^1 -solution of (3.1).

Evidently, if $B(y)$ is invertible in a neighborhood of $y^0 = \varphi^{-1}(x^0)$ then (3.9) satisfies the conditions of Definition 2.1 and the augmentation procedure of Section 2 can be applied. This is the case when (3.1) has index 1 in the sense of the following definition:

Definition 3.2. *The quasilinear system (3.1) is a nonsingular DAE of index 1 if*

$$(3.10) \quad \{x \in W, G(x) \in \text{rge } A(x)|_{T_x W}\} \Rightarrow \text{rank } A(x)|_{T_x W} = \text{rank } A(x) (= r).$$

From (3.10) it follows that $B(y^0) \in GL(\mathbb{R}^r, \text{rge } A(x^0))$ and $D\varphi(y^0) \in GL(\mathbb{R}^r, T_{x^0} W)$ and this provides the basis of the following existence and uniqueness theorem for (3.1):

Theorem 3.1. *Let (3.1) be a nonsingular DAE of index 1. Then, for any $x^0 \in W_1 = \pi(TW \cap M) \subset W$ there exists a unique C^1 solution $x : J \rightarrow \mathcal{D}$ on some open interval J containing the origin, of the initial value problem*

$$(3.11) \quad A(x)\dot{x} = G(x), \quad x(0) = x^0.$$

Moreover, no C^1 solution of (3.11) exists for $x^0 \notin W_1$.

Definition 3.2 does not rule out the existence of points $x^0 \in W$ where $\text{rank } A(x^0)|_{T_{x^0} W} < r$. Such points do not belong to the set $W_1 = \pi(TW \cap M)$ and hence no C^1 solution to the corresponding initial value problem (3.11) exists. Nevertheless, in analogy to Definition 2.3 'one-sided' solutions may well occur at such points:

Definition 3.3. A solution of the initial value problem (3.11) at a point $x^0 \notin \pi(TW \cap M)$ is any continuous function $x : J \rightarrow \mathcal{D}$ defined on an interval of the form $J = [0, T)$ or $J = (-T, 0]$ for some $T > 0$ which is of class C^1 on $J^0 = J \setminus \{0\}$ and satisfies $x(t^*) = x^*$ and $A(x(t))\dot{x}(t) = G(x(t))$ for $t \in J^0$.

In [RR92] a precise definition of accessible and inaccessible impasse points of nonsingular DAE's of index 1 (and higher) is given where the existence of one-sided solutions can be guaranteed. We shall not repeat this theory here but summarize the main result in the form of the following theorem: (see [RR92], Lemma 5.1 and Theorem 5.1):

Theorem 3.2. Let (3.1) be a nonsingular DAE with index 1. The point $x^0 \in W$ is an accessible or inaccessible impasse point of (3.1) if and only if $\xi_0 = \varphi^{-1}(x^0)$ is an accessible or inaccessible standard singular point, respectively, of the reduction (3.9) of (3.1) locally near x^0 . Then, the initial value problem (3.11) has exactly two solutions in the sense of Definition 3.3, both defined either on $J = [0, T)$ or $J = (-T, 0]$ for some $T > 0$. Moreover, $\|\dot{x}(t)\|$ tends to infinity as t tends to zero.

Because C^1 -solutions of a (not necessarily nonsingular) DAE (3.1) lie in $W_1 = \pi(W \cap TM)$, their closure relative to the open set $\mathcal{V} \subset \mathbb{R}^r$ must lie in W when W is closed in \mathcal{D} . This is the case in many practical applications but, mathematically, it is not the only possibility. When W is not closed in \mathcal{D} it becomes possible for points $x^0 \notin W$ to be reached in finite time by C^1 -trajectories that cannot be continuously extended beyond x^0 . Likewise, there may be points $x^0 \in W$ corresponding to higher singularities of the reduction; that is, with $\dim \ker B(y^0) > 1$, at which C^1 trajectories stop.

As an illustration we consider the first and third example of [CD89] which have the form

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \dot{x} = G_j(x), \quad x \in \mathbb{R}^3, \quad j = 1, 2$$

with

$$G_1(x) = \begin{pmatrix} x_3 \\ x_3 \\ x_1 + x_3(x_2 + x_3^2) \end{pmatrix}, \quad G_2(x) = \begin{pmatrix} x_3^2 \\ -x_3 \\ x_1 + x_3(x_2 + x_3^2) \end{pmatrix}$$

Hence, in both examples the conditions of Definition 3.1 are satisfied with $r = 2$. Moreover, we have

$$W = \{x \in \mathbb{R}^3 : x_1 + x_3(x_2 + x_3^2) = 0\},$$

and, evidently, the mapping

$$\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}^3, \quad \varphi(y) = \begin{pmatrix} y_2(y_1 + y_2^2) \\ -y_1 \\ -y_2 \end{pmatrix}, \quad D\varphi(y) = \begin{pmatrix} y_2 & y_1 + 3y_2^2 \\ -1 & 0 \\ 0 & -1 \end{pmatrix}$$

is here a global diffeomorphism from \mathbb{R}^2 onto W . Therefore, with the linear isomorphism

$$L^0 P^0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

the reductions of the two problems have the form

$$\begin{pmatrix} y_2 & y_1 + 3y_2^2 \\ -1 & 0 \end{pmatrix} \dot{y} = H_j(y), \quad j = 1, 2$$

where

$$H_1(y) = \begin{pmatrix} -y_2 \\ -y_2 \end{pmatrix}, \quad H_2(y) = \begin{pmatrix} y_2^2 \\ -y_2 \end{pmatrix}.$$

Obviously, in both cases, the singular points form the one-dimensional manifold

$$K = \{y \in \mathbb{R}^2 : y_1 + 3y_2^2 = 0\}$$

and we have $\dim \ker B(y^*) = 1$ and $\text{rge } B(y^*) = \text{span } (y_2^*, -1)^T$ for $y^* \in K$. Moreover, for $j = 1$ we see that $H_1(y^*) \notin \text{rge } B(y^*)$ for all $y^* \in K$ with $y_2^* \neq -1$ while for $j = 2$ we have $H_2(y^*) \in \text{rge } B(y^*)$ for all $y^* \in K$. Thus, in the second case, none of the points of K is a standard impasse point. On the other hand, for $j = 1$, a simple calculation with $u = (0, 1)^T \in \ker B(y^*)$ and $v = (1, y_2^*)^T \in \ker B(y^*)^T$ shows that

$$\alpha(y^*)(u, v) = -6(y_2^*)^2(y_2^* + 1),$$

whence, all points $y^* \in K$ with $y_2^* \neq 0, -1$ are here standard impasse points which are accessible for $y_2^* > -1$, $y_2^* \neq 0$ and inaccessible for $y_2^* < -1$.

Thus, for $j = 1$ the points $y^* \in K$, $y_2^* = 0, -1$ and for $j = 1$ all points $y^* \in K$ are higher singularities. In both cases, $y^* = 0$ is also a stationary point. The differences between these higher singularities and the standard impasse points in the first example were observed in [CD89] but explained differently.

4. Computation of Singular Points of DAE's.

The reduction process for quasilinear DAE's sketched in the previous section and the resulting theory of impasse points for nonsingular DAE's of index 1 suggests that we may compute such points by applying the augmentation approach of Section 2 to the reduced system (3.9). In this section we show that this does indeed lead to an efficient computational algorithm.

For simplicity we develop the method only for DAE's of the following form occurring frequently in applications:

$$(4.1) \quad \begin{pmatrix} A_1(x) \\ 0 \end{pmatrix} \dot{x} = \begin{pmatrix} G_1(x) \\ G_2(x) \end{pmatrix}.$$

Here $A_1 : \mathcal{D} \rightarrow \mathcal{L}(\mathbb{R}^r)$, $G_1 : \mathcal{D} \rightarrow \mathbb{R}^r$, $G_2 : \mathcal{D} \rightarrow \mathbb{R}^\rho$ are C^2 -maps on some open set $\mathcal{D} \subset \mathbb{R}^n$, with $n = r + \rho$, $\rho > 0$, and (4.1) is assumed to be a quasilinear DAE in the sense of Definition 3.1.

The submersion condition for the mapping (3.3) requires that $\text{rank } DG_2(x) = \rho$ for $x \in \mathcal{D}$ and hence that the set

$$(4.2) \quad N = \{x \in \mathcal{D} : G_2(x) = 0\}$$

is an r -dimensional C^2 -submanifold of S .

The manifolds (3.5) and (3.6) are here given by

$$(4.3) \quad M = \{(x, p) \in \mathcal{D} \times \mathbb{R}^n : x \in N, A_1(x)p = G_1(x)\}$$

$$(4.4) \quad W = \{x \in N : \text{rank } A_1(x) = r\}.$$

and this allows for a considerable simplification of the reduction process. As in [Rh86] we introduce at any "current" point $x_c \in N$ a tangential local coordinate system. For this let $U^c = U(x_c) \in \mathcal{L}(\mathbb{R}^r, \mathbb{R}^n)$ define an orthonormal basis of $\ker DG_2(x_c)$. Then the implicit function theorem applied to the equation

$$(4.5) \quad G_2(x_c + U^c y + DG_2(x_c)^T z) = 0, \quad y \in \mathbb{R}^r, \quad z \in \mathbb{R}^p$$

guarantees the existence of open neighborhoods \mathcal{U}_c of the origin of \mathbb{R}^r and $\mathcal{V}_c \subset \mathbb{R}^n$ of x_c such that for any $y \in \mathcal{U}_c$ there exists exactly one solution z of (4.5) with $x_c + U^c y + DG_2(x_c)^T z \in \mathcal{V}_c$ and that the mapping $\psi : \mathcal{U}_c \mapsto \mathbb{R}^p$, $\psi(y) = z$ is of class C^1 on \mathcal{U}_c . Evidently, we have $\psi(0) = 0$ and $D\psi(0) = 0$ and

$$(4.6) \quad \Phi : \mathcal{U}_c \mapsto \mathbb{R}^n, \quad \Phi(y) = x_c + U^c y + DG_2(x_c)^T \psi(y), \quad \forall y \in \mathcal{U}_c,$$

is a diffeomorphism from \mathcal{U}_c onto $N \cap \mathcal{V}_c$. In other words, Φ^{-1} is a chart of N at x_c and we call Φ a tangential local coordinate map at x_c .

As in [Rh88], by shrinking if necessary the neighborhoods \mathcal{U}_c and \mathcal{V}_c , we can extend $U^c = U(x_c)$ to a moving frame on \mathcal{V}_c ; that is, to a C^1 -mapping $U : \mathcal{V}_c \rightarrow \mathcal{L}(\mathbb{R}^r, \mathbb{R}^n)$ such that the columns of $U(x)$ form an orthonormal basis of $\ker DG_2(x)$ for each $x \in \mathcal{V}_c$.

Then, for $y \in \mathcal{U}_c$ and $x = \Phi(y)$ we have $(x, p) \in M$ exactly if

$$(4.7) \quad \begin{aligned} B(y)p &= H(y) \\ B(y) &= A_1(\Phi(y))D\Phi(y), \quad H(y) = G_1(\Phi(y)). \end{aligned}$$

Hence, if $x_c \in W$ then necessarily $\text{rank } A_1(x) = r$ for $x \in \mathbb{R}^n$ in some neighborhood of x_c and thus, by restricting again, if needed, the neighborhoods \mathcal{U}_c and \mathcal{V}_c we find that (4.7) represents for $y \in \mathcal{U}_c$ the reduction of (4.1) locally near x_c .

For the computation we need to be able to evaluate $\Phi(y)$ and $D\Phi(y)$ for $y \in \mathcal{U}_c$. There are various possibilities for computing $x = \Phi(y)$ for given y . For example, as discussed in

[Rh88], we may use the QR-factorization

$$(4.8) \quad DG_2(x_c)^T = (Q_1, Q_2) \begin{pmatrix} R \\ 0 \end{pmatrix}$$

where $\text{rge } Q_2 = \ker DG_2(x_c)^T$ and then set $U^c = Q_2$. Now, for any given $y \in \mathbb{R}^r$ with sufficiently small norm the chord Newton algorithm

Eval Φ : **Input:** x, R, Q_1

while 'no convergence'

 solve $R^T z = G_2(x)$ for z ;

 set $x := x - Q_1 z$;

Output: x .

converges to $\Phi(y) \in N$ and hence implements the tangential coordinate system.

For the computation of $D\Phi(y)$ at any $y \in \mathcal{U}_c$ note that

$$(4.9) \quad (U^c)^T D\Phi(y) = (U^c)^T U^c + (U^c)^T DG_2(x_c)^T D\psi(y) = I_r.$$

Moreover, because of $DG_2(\Phi(y))D\Phi(y) = 0$ it follows that $D\Phi(y) = U(\Phi(y))K(y)$ for some nonsingular $K(y) \in \mathcal{L}(\mathbb{R}^r)$. Together with (4.9) this implies that $K(y) = U(\Phi(y))^T D\Phi(y)$ and therefore that

$$(4.10) \quad D\Phi(y) = U(\Phi(y))(U^c)^T U(\Phi(y))^{-1}.$$

Clearly, since $U : \mathcal{V}_c \rightarrow \mathcal{L}(\mathbb{R}^r, \mathbb{R}^n)$ is of class C^1 , the same holds for $D\Phi$. But it turns out that we do not need $U(x)$ to be a C^1 -moving frame on a neighborhood of x_c on N . In fact, suppose that $\hat{U}(x) \in \mathcal{L}(\mathbb{R}^r, \mathbb{R}^n)$ represents for $x = \Phi(y)$, $y \in \mathcal{U}_c$, an arbitrary basis matrix of $\ker DG_2(x)$ and that $\hat{U}(x_c) = U(x_c)$. Then we have $U(x) = \hat{U}(x)Q(x)$ with some nonsingular $Q(x) \in \mathcal{L}(\mathbb{R}^r)$ and hence

$$(4.11) \quad \begin{aligned} D\Phi(y) &= U(x)((U^c)^T U(x))^{-1} = \hat{U}(x)Q(x)((U^c)^T \hat{U}(x)Q(x))^{-1} \\ &= \hat{U}(x)((U^c)^T \hat{U}(x))^{-1}. \end{aligned}$$

While for points x in a neighborhood of a fixed point x_c the particular choice of the basis matrix $U(x)$ does not matter, the orientation of $U(\tilde{x}_c) \equiv \tilde{U}^c$ does play a role when we move from x^c to another “current” point \tilde{x}_c . The compatibility condition for charts on a C^1 manifold requires at least that $\tilde{U}^c = U(\tilde{x}_c)$ tends to $U^c = U(x_c)$ when \tilde{x}_c converges to x_c . This can be guaranteed by applying the moving frame algorithm of [Rh88] in the construction of the new basis \tilde{U}_c . However, when (4.1) is a nonsingular DAE of index 1 and hence when one of the augmentation procedures of section 2 can be applied to the reduced system (4.7), then it suffices to ensure that both bases have the same orientation; that is, that

$$(4.12) \quad \det (\tilde{U}^c)^T U^c > 0.$$

This is certainly ensured by the moving frame algorithm. But in practice, it was found advantageous to apply a simpler heuristic procedure. Let $u^c = U^c(1, 1, \dots, 1)^T$ be the “diagonal” vector of the positive octant of the basis U^c . Suppose that a new basis matrix \tilde{U}^c has been computed with the columns $\tilde{u}^1, \dots, \tilde{u}^r$. Then we replace the vector \tilde{u}^i by $-\tilde{u}^i$ whenever $(u^c)^T \tilde{u}^i \leq 0$ for any $i = 1, \dots, r$. This certainly guarantees that (4.12) holds for the modified basis.

As indicated, if (4.1) is a nonsingular DAE of index 1 then one of the augmentation procedures of section 2 will be applied to the reduced ODE (4.7). In practice, it is useful to work with a larger augmentation (2.14) rather than with (2.8) in order for the process to function also near higher order singularities than just standard impasse points. For this the augmentation (2.22) with $q = 2$ was chosen for which $v(y)$ and $\gamma(y)$ are easily determined by (2.23).

For the solution of (4.1) subject to some initial condition $x(0) = x^0 \in N$ the augmentation is constructed at certain computed points x_c along the trajectory. At these points the local coordinate map (4.6) is obtained and hence the reduced system (4.7) has the form

$$B^c p = H^c, \quad B^c = A_1(x_c)U^c, \quad H^c = G_1(x_c)$$

There are various ways for computing suitable vectors b, c_1, c_2 to ensure that the matrix of the augmented system (2.22); that is, here

$$(4.13) \quad \begin{pmatrix} B^c & -H^c & e \\ c_1^T & 0 & 0 \\ c_2^T & 0 & 0 \end{pmatrix} \begin{pmatrix} v_1 & v_2 \\ w_1 & w_2 \\ z_1 & z_2 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix},$$

is nonsingular. For relatively small dimensions r we may use, for instance, the singular value decomposition

$$(4.14) \quad \begin{cases} V_L^T(B^c, -H^c)V_R = (\Sigma, 0), \\ V_L \in \mathbb{R}^{r \times r}, \quad V_R \in \mathbb{R}^{r+1 \times r+1}, \quad \Sigma = \text{diag}(\sigma_1, \dots, \sigma_r). \end{cases}$$

Let $e_k^m, k = 1, \dots, m$, denote the natural unit-basis vectors of \mathbb{R}^m . Then, with

$$V_R e_{r+1}^{r+1} = \begin{pmatrix} u_1 \\ \omega_1 \end{pmatrix}, \quad V_R e_r^{r+1} = \begin{pmatrix} u_2 \\ \omega_2 \end{pmatrix}$$

we choose the augmenting vectors

$$(4.15) \quad e = \pm V_L e_r^r, \quad c_1 = \frac{u_1}{\|u_1\|_2}, \quad c_2 = \frac{u_2}{\|u_2\|_2},$$

where the sign of e will be addressed shortly. Under the assumption that $\text{rank}(B^c, -H^c) \geq r-1$, the matrix of (4.13) is nonsingular if and only if $\omega_1^2 + \omega_2^2 \neq 1$. In fact, for any null-vector $w = (q^T, \xi, \eta)^T \in \mathbb{R}^{r+2}$ of (4.13) we have

$$(4.16) \quad \sigma_i \bar{q}_i = 0, \quad i = 1, \dots, r-1, \quad \sigma_r \bar{q}_r + \eta = 0, \quad \text{for} \quad \begin{pmatrix} \bar{q} \\ \bar{\xi} \end{pmatrix} = V_R^T \begin{pmatrix} q \\ \xi \end{pmatrix},$$

Hence, in the case of $\text{rank}(B^c, -H^c) = r$ we see that $\sigma_r > 0$ and therefore that $\eta = 0$ whence $q = \lambda u_1, \xi = \lambda \omega_1$ and $0 = c_1^T q = \lambda$; that is, $w = 0$. When the rank of $(B^c, -H^c)$ is $r-1$ then (4.16) implies that $\bar{q} = \bar{q}_r e_r^r$ and therefore that

$$0 = u_1^T q = \bar{q}_r u_1^T u_2 + \bar{\xi} u_1^T u_1,$$

$$0 = u_2^T q = \bar{q}_r u_2^T u_2 + \bar{\xi} u_2^T u_1,$$

where, because of the orthonormality of the vectors $V_R e_{r+1}^{r+1}$ and $V_R e_r^{r+1}$ the determinant of the matrix equals $\omega_1^2 + \omega_2^2 - 1$. Hence, if this determinant is nonzero then we have again $w = 0$ while, it is readily seen, that in the case of a zero determinant the matrix may indeed be singular. Note that $\text{rank}(B^c, -H^c) \geq r - 1$ obviously holds not only at standard impasse points x_c .

For the choice of the direction of the vector e of (4.15) suppose that B^c is nonsingular; that is, that we are not exactly at a singular point of the reduced system. Then a block LU-factorization of the matrix of (4.13) shows that

$$(4.17) \quad \det \begin{pmatrix} B^c & -H^c & e \\ c_1^T & 0 & 0 \\ c_2^T & 0 & 0 \end{pmatrix} = \det B^c \det (c_1, c_2)^T (B^c)^{-1} (H^c, -e).$$

The solution of the augmented system (4.13) gives

$$(4.18) \quad I_2 = (c_1, c_2)^T (v_1, v_2) = (c_1, c_2)^T (B^c)^{-1} (H^c, -e) \begin{pmatrix} w_1 & w_2 \\ z_1 & z_2 \end{pmatrix}.$$

In accordance with (2.23) we compute now

$$(4.19) \quad v^c = \begin{pmatrix} w_1 & w_2 \\ z_1 & z_2 \end{pmatrix}^{-1} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad \gamma^c = \det \begin{pmatrix} w_1 & w_2 \\ z_1 & z_2 \end{pmatrix}.$$

Thus (4.17 - 19) imply that

$$(4.20) \quad \text{sign det} \begin{pmatrix} B^c & -H^c & e \\ c_1^T & 0 & 0 \\ c_2^T & 0 & 0 \end{pmatrix} = \text{sign det } B^c \text{ sign det } \gamma^c.$$

In line with the theory of section 2 we choose the augmenting vector e such that the left side of (4.20) remains positive. In other words, we use the factorization of the matrix of the augmented system (4.13) to monitor the sign of its determinant and replace the computed z_1 and z_2 by their negative values when that determinant is negative.

For the computation of the solution of (4.1) with the initial condition $x(0) = x^0$ we use a standard explicit Runge-Kutta solver such as RKF-45. The algorithm for one step along the solution of (4.1) then has the general form:

SingDAE: **Input:** Current point x_c , tolerance tol ,
 suggested step h ; minimal step h_{min} , step counter k ;

- 1 Compute the QR-factorization (4.8), set $U^c = Q_2$ and $y_c = 0$;
- 2 With $B(y_c) = A_1(x_c)U^c$ compute the augmentation vectors (4.13);
- 3 Solve the augmented system (2.17) to obtain $\gamma^c = \gamma(x_c)$;
4. Take a Runge Kutta step for (2.12) with y_c , h , tol to obtain y^n , h_{new} ;
5. **If** 'Step not accepted' **then**
 replace h by $h/2$ and for $|h| \geq h_{min}$ go to 2, otherwise **error return**;
6. Step acceptable: Call **Eval- Φ** to obtain $x^n = \Phi(y^n) \in N$;
8. Use (4.10) to compute $D\Phi(y^n)$ and $B(y^n) = A_1(x^n)D\Phi(y^n)$;
9. Solve the augmented system (2.17) to obtain γ^n
10. **Output** $k = k + 1$, $h = h_{new}$, x^n , γ^c , γ^n ;
11. **If** 'sign $\gamma^c \neq \text{sign } \gamma^n$ ' **then**
 singular point passed, if desired, call root finder to compute the point.

The Runge Kutta solver in step 4. requires a subroutine for computing the right hand $v(y)$ of the reduced explicit equation (4.7). This is handled by a subroutine of the form:

Eval v: **Input:** Q_1 , and R , y ;

1. Use **Eval- Φ** to compute $x = \Phi(y)$;
2. Use (4.10) to compute $D\Phi(y)$ and $B(y) = A_1(x)D\Phi(y)$;
3. Form the augmented system (2.17) and solve;
4. Use (2.18) to compute $v(y)$ and $\gamma(y)$;
5. **Output:** $v(y)$, $\gamma(y)$.

When γ has different sign at two consecutive points, say, x^k and x^{k+1} , indicating the presence of a singular point, then a root finder can be applied to determine the step h from x^k which gives $\gamma(y) = 0$ and hence which provides the singular point. For this a simple algorithm of the Dekker-Brent type (see [B73]) has been used. If a standard impasse point has been passed then x^k and x^{k+1} lie on trajectories with opposite orientation. Hence, in order to proceed from x^{k+1} , we have to change the sign of the step h . At higher order singular points this may or may not be required.

The routine 'SingDae' computes a new augmentation for each Runge Kutta step. This has been found adequate in smaller applications. However, for larger problems it is desirable to retain the same augmentation for several Runge Kutta steps. For this the condition of the linear augmented system may be monitored. This is easily done in step 4 of 'Eval v' or in step 9. of 'SinDae Step'. An additional check is the rate of convergence of the chord-Newton process of 'Eval Φ '. Whenever one of these tests indicates that the augmentation has become unreliable then the output of 'SingDae' is not accepted and the routine is restarted with a new augmentation.

There should be no need to enter into the details of such a modification of the process. The approach is similar to that employed in [PR91].

5. Numerical Examples.

As noted in the introduction, impasse points for DAE's arise frequently in nonlinear circuit problems. As an example we consider a simple circuit consisting of a nonlinear resistor, linear capacitor, and linear inductor in parallel. The characteristic of the resistor is given by $u = \gamma + i^2$ where i and u denote the corresponding branch current and voltage drop, respectively. The example was considered earlier by F. Takens (see [T76]) and again in [RR92] and is modelled by the DAE

$$(5.1) \quad \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \dot{x} = \begin{pmatrix} x_4 \\ x_2 \\ x_1 + x_2 + x_3 \\ x_1 - \gamma - x_1^2 \end{pmatrix}$$

Here $x_j = i_j$, $j = 1, 2, 3$, are the currents in the three branches, $x_4 = u$ is the voltage drop, and, for simplicity, the capacitance and inductance were normalized to one. It is readily verified that (5.1) is a DAE on all of \mathbb{R}^4 with $r = 2$ in the sense of Definition 3.1.

In the notation of (4.1) the constraint manifold (4.2) is here given by

$$(5.2) \quad N = \{x \in \mathbb{R}^4 : G_2(x) = 0\}, \quad G_2(x) = \begin{pmatrix} x_1 + x_2 + x_3 \\ x_4 - \gamma - x_1^2 \end{pmatrix}.$$

In this case we can define the following global coordinate mapping on N

$$(5.3) \quad \Phi : \mathbb{R}^2 \rightarrow N, \quad \Phi(y) = \begin{pmatrix} y_1 \\ y_2 \\ -(y_1 + y_2) \\ \gamma + y_1^2 \end{pmatrix}.$$

and hence the system

$$(5.4) \quad \frac{1}{3} \begin{pmatrix} -1 & -1 \\ 2y_1 & 0 \end{pmatrix} \dot{y} = \begin{pmatrix} \gamma + y_1^2 \\ y_2 \end{pmatrix},$$

constitutes a (global) reduction of (5.1).

Clearly, (5.4) is a nonsingular ODE for all $y \in \mathbb{R}^2$ with $y_1 \neq 0$. Moreover, all points of $\{y \in \mathbb{R}^2 : y_1 = 0, y_2 \neq 0\}$ are standard singular points of (5.4) while at $y = 0$ the condition (2.3) is violated. Thus (5.1) has the one-dimensional submanifold $\{x \in \mathbb{R}^4; x = (0, \xi, -\xi, \gamma)^T, \xi \in \mathbb{R}, \xi \neq 0\}$ of standard impasse points while $x^* = (0, 0, 0, \gamma)^T$ is a higher singularity.

A closer analysis of the example in [RR92] shows that the singularity at x^* has a different character for the four cases (i) $\gamma > 1/8$, (ii) $1/8 \geq \gamma > 0$, (iii) $\gamma = 0$, (iv) $\gamma < 0$. In particular, for (ii) - (iv) the point x^* is a funnel point (see [T76]).

Figures 1 - 3 show computed results obtained with the algorithm of Section 4 for the three values $\gamma = 1.0, 0.0625, -1.0$. In each case the impasse points $x = (0, \xi, -\xi, \gamma)^T$ for $\xi > 0$ are accessible while those for $\xi < 0$ are inaccessible. Moreover, for $\gamma = -1.0$

the funnel-nature of x^* is clearly visible, but recall that at x^* the derivative \dot{x} becomes infinite and hence no C^1 -solution passes through that point. The results certainly show that already very simple circuits may have a relatively complex singularity behavior.

As a second example we consider a two-phase plug flow problem described by Byrne and Hindmarsh ([BH87], see also [HLR89]). The equations are given in the form:

$$\begin{aligned} & \pi \sqrt{\frac{R}{2\rho}} (R - y)^2 \sqrt{-P'} (2.5 \log[\sqrt{\frac{\rho R}{2}} \frac{y}{\mu} \sqrt{-P'} - 5] + 10.5) \\ & \quad - bQ_{c0} - \frac{P_0}{P} Q_{c0} (1 - b) = 0, \\ & 2\pi \sqrt{\frac{R}{2\rho}} \sqrt{-P'} ((2.5Ry - 1.25y^2) \log[\sqrt{\frac{\rho R}{2}} \frac{y}{\mu} \sqrt{-P'} - 5] \\ & \quad + 3Ry - 2.125y^2 - 13.6R\mu \sqrt{\frac{2}{\rho R}} \frac{1}{\sqrt{-P'}}) - Q_a = 0, \end{aligned}$$

where P' is the time-derivative of P . With $x_1 = P$, $x_2 = 1/\sqrt{-P'}$, and $x_3 = y\sqrt{-P'}$ these equations become

$$\begin{aligned} & x_2^2 x_1' + 1 = 0 \\ (5.5) \quad & x_1(4.2 + \log(c_1 x_3 - 5))(1 - x_2 x_3)^2 - c_2 x_2 (b x_1 + c_4(1 - b)) = 0 \\ & x_3((2 - x_2 x_3) \log(c_1 x_3 - 5) + (2.4 - 1.7 x_2 x_3) - c_3 = 0. \end{aligned}$$

Here, after scaling the time by a factor 10^{-7} , the constants are

$$c_1 = \frac{R}{\mu} \sqrt{\frac{\rho R}{2}}, \quad c_2 = \frac{\rho Q_{c0}}{2.5\pi\mu R c_1}, \quad c_3 = \frac{10.88}{c_1} + \frac{0.4\rho Q_a}{\pi\mu R c_1}, \quad c_4 = 10^{-7} P_0$$

As in [HLR89] we used the values

$$\begin{aligned} & R = 45.72, \quad \rho = 0.814, \quad \mu = 0.098, \quad b = 0.345, \\ & Q_{c0} = 1.7153 \times 10^6, \quad Q_a = 3.027 \times 10^5, \quad P_0 = 1.378 \times 10^8 \end{aligned}$$

for which

$$c_1 = 2012.47, \quad c_2 = 19.7157, \quad c_3 = 3.48464, \quad c_4 = 13.78$$

It turns out that the system (5.5) has a singularity at $x^* = (0, 0, x_3^*)^T$, with $x_3^* = 0.236849$. More specifically, the system has index one in the sense of Definition 3.2 and for the reduced ODE, x^* is a basic 1-singular point. But, since the form (2.6) is zero at x^* , this point is not a standard singular point. In fact, x^* corresponds to a hysteresis point for stationary equations.

The code was applied to the system (5.5) starting from the point

$$y^0 = (13.78, 0.42256012, 0.24921339)^T$$

given in [HLR89]. The resulting trajectory is shown in Figure 4. The singularity y^* is reached for $t^* = 1.0958$ where the derivative y' becomes infinite. At the singular point the flow is choked and hence the part of the trajectory beyond that point is physically meaningless. But it is noteworthy that the code has no difficulty in passing through that point.

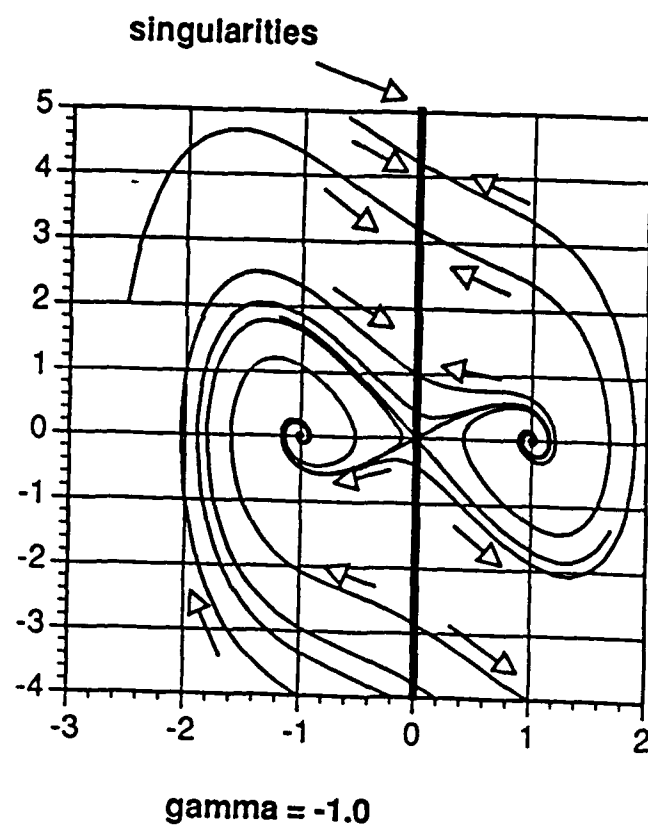


FIGURE 3.

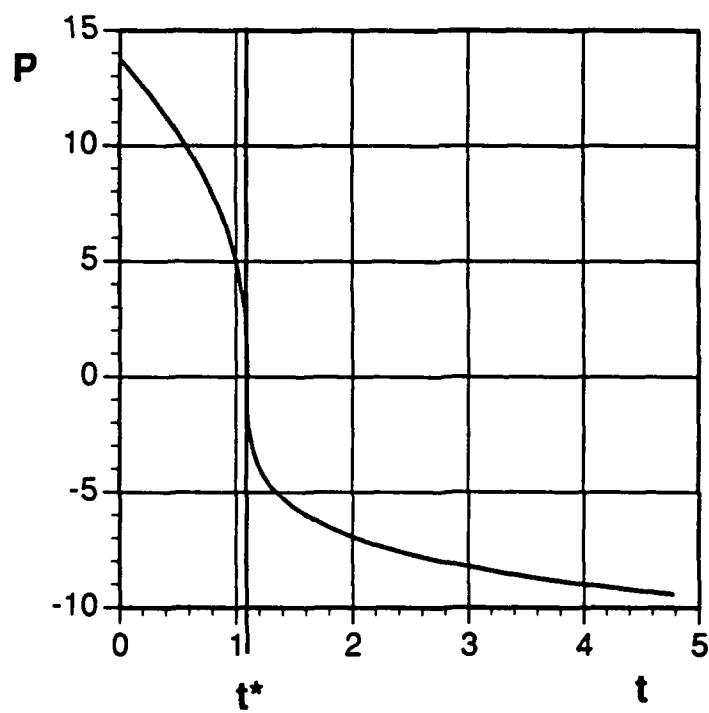


FIGURE 4.

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